Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -93.1 °C

Global applicability domain: Inside

Local applicability domain index: 9.35e-01

Confidence level: 7.24e-01

Nearest Neighbors from the Training Set

Image not found
2,6-Octadiene, 4,5-dimethyl-
Measured: -64.8
Predicted: -103

Image not found
1,5-Heptadiene, 2,6-dimethyl-
Measured: -70.0
Predicted: -74.7

Image not found
1,6-Heptadiene
Measured: -129
Predicted: -132

Image not found
2-Methylhexa-1,5-diene
Measured: -129
Predicted: -112

Image not found
5-Undecyne
Measured: -74.1
Predicted: -62.6